EOS MLS v2.2 Data Quality Document (Short Version)

The Earth Observing System (EOS) Microwave Limb Sounder (MLS) team has started reprocessing using version 2.20 MLS algorithms. This is the 2nd major MLS data release (version 1.51/1.52 being the first).

Reprocessing of selected days in 2004, 2005, and 2006 is in progress with initial priority being given to validation results of special interest to the MLS team. A calendar of reprocessed and planned days for the early v2.20 reprocessing phase is available via the MLS homepage at http://mls.jpl.nasa.gov. "Forward processing" of incoming MLS data with v2.20 is planned to commence in February/March 2007. The reprocessed data are initially being provided to the Aura validation community via the Aura Validation Data Center (AVDC). For most species the results are generally very similar to the provisional version 2.10 data set (only a few days processed) that had been made available for the September 2006 Aura meeting; results differ somewhat more (from v2.10) for H2O and N2O.

The main changes between v2.20 and the earlier v1.5 data are described below. More details will be given in validation papers to be submitted in the spring of 2007. A more detailed v2.2 data quality document will also be released in spring 2007 when the data are made publicly available at the GSFC DAAC.

The v2.20 algorithms produce temperature, H2O, and relative humidity (RHi) data with higher vertical resolution than in v1.5. Version 2.20 shows significant improvements over version 1.5 in the CO product (upper troposphere and throughout the middle atmosphere), and displays a significant reduction of previously identified high biases in stratospheric HNO3. Some changes to calibration, spectroscopy, and forward model / retrieval configurations have also taken place. The vertical range of useful retrievals has increased for some products. The v2.20 retrievals use GMAO GEOS-5 temperature data as part of the production stream. Stratospheric column abundances are now reported only for ozone (see the stratospheric ozone section below).

Detailed information on specific products, including useful vertical ranges and preliminary data screening rules, are given below. As in version 1.5, data should only be used when the corresponding precision values are positive, when the 'Status' flag is an even number (or more strictly equals zero for some upper tropospheric products), and when the 'Quality' field is greater than a stated threshold. A new field called 'Convergence' gives additional information on data quality which should be considered for some products as described below. 'Convergence' is the ratio of the chi-squared value achieved in the retrieval to that

expected, with values of 1.0-1.1 typically indicating good convergence. An additional bit (value 64) has been added to the 'Status' field to indicate situations where GEOS-5 temperatures were not available to be used as a-priori information. All the data screening rules given below are preliminary and may be revised at a later date.

Version 2.20 data users are strongly advised to contact the MLS scientists responsible for their products of interest for further information. Users can register for updates on MLS operations and data at the MLS website.

PRODUCT-SPECIFIC COMMENTS

Temperature

- Responsible scientist: Michael Schwartz (michael@mls.jpl.nasa.gov)
- Useful range: 316 - 0.001 hPa

Vertical resolution for temperature in the upper troposphere has been improved from about 8 km to 5 km, through the use of isotopic O2 (band 8) radiances and temperature is now retrieved on a 12 levels per decade vertical grid between 1000 and 22 hPa. Vertical resolution in the upper stratosphere is somewhat degraded compared to v1.5 (due to changes in the use of radiances), being about 4 km at 31 hPa up to 8 km at 1 hPa. Biases with respect to the GEOS-5 a priori are somewhat oscillatory with height. V2.2 average temperatures are lower by 0 to 4 K than for v1.5 in the stratosphere and lower mesosphere, which makes them 0 to 2 K lower than the GEOS-5 a priori in the lower stratosphere, and 0 to 5 K higher in the upper stratosphere.

- Data screening:

Only use profiles with even values of the Status field and positive precision values, as well as Quality field > 0.5. There is no obvious correlation between the behavior of the temperature product and the Quality or Convergence flags. However, it is recommended that Quality < 0.5 be excluded from scientific studies, as low quality indicates a poor radiance fit. This recommendation is preliminary and may change. Use of this value excludes approximately 3% of the profiles.

Geopotential Height (GPH)

- Responsible scientist: Michael Schwartz (michael@mls.jpl.nasa.gov)
- Useful range: 316 - 0.001 hPa

V2.2 GPH is typically within 60m of v1.5 GPH at 316 hPa and within 10 m at 100 hPa. The general cold bias of v2.2 temperature relative to v1.5 in the stratosphere and lower mesosphere results in a relative bias in GPH which increases with height, such that the v2.2 0.1 hPa surface is typically 600m lower than that of v1.5.

- Data screening:

Recommendations regarding screening for Status, precision, and Quality for GPH are identical to those for temperature.

CO (stratosphere and mesosphere)

- Responsible scientist: Hugh Pumphrey (H.C.Pumphrey@ed.ac.uk)
- Useful range: 215 - 0.0046 hPa

CO values above 60 km have decreased considerably due to a fix in the calibration of band 25 (digital autocorrelator spectrometer or DACS) radiances at Level 1. CO profiles are now considerably less jagged throughout the middle atmosphere. This was achieved partly through the use of tighter a priori errors and by the improved handling of DACS radiances.

- Data Screening:

Only use profiles with even values of Status and positive precision values, and with Quality > 0.2 and Convergence < 1.8. Quality is not very well correlated with obviously bad profiles and usually lies between 1.5 and 3; we recommend rejecting values below 0.2 as a precaution. Convergence values should be close to 1; values > 1.8 are nearly always associated with clearly bad chunks and should always be rejected.

CO (upper troposphere, pressures of 100 hPa and larger)

- Responsible scientist: Nathaniel Livesey (livesey@mls.jpl.nasa.gov)
- Useful range: 215 hPa to 100 hPa (not always in upper troposphere)

The v2.2 upper tropospheric CO product shows significantly less scatter than seen in v1.5 (mainly associated with situations of thick cloud). However, the underlying factor of roughly 2 high bias at 215 hPa

generally remains. As with v1.5, the v2.2 upper tropospheric CO data are currently only recommended for use at pressures of 215 hPa and less.

- Data screening:

The same quality control screening rules recommended for v1.5 should be used for v2.2, except that the threshold value (lower limit) for Quality should be 1.2 (a preliminary value based on a limited number of reprocessed days), and data where 'Convergence' is greater than 1.8 should be rejected (as for the stratosphere). As with v1.5, we currently only recommend MLS upper tropospheric CO data where the Status field is zero, (i.e., discarding profiles possibly contaminated by clouds). This rule may be overly cautious, leading to about 30% of tropical profiles being discarded. Further investigations may result in less draconian quality screening rules, to be described in the validation papers and the full data quality document.

O3 (upper troposphere, pressures of 100 hPa and larger)

- Responsible scientist: Nathaniel Livesey (livesey@mls.jpl.nasa.gov)
- Useful range: 215 hPa to 100 hPa (not always in upper troposphere)

The v2.2 upper tropospheric O3 product is broadly similar to the v1.5 product. The amount of scatter due to cloud contamination has been reduced. Biases in these data compared to sondes and other observations will be reported in the validation papers.

- Data screening:

Only use profiles with Status = 0 and positive precision values, and with Quality > 1.2, and Convergence < 2. The Quality threshold has changed from v1.5. The Status rule above discards profiles possibly contaminated by clouds. This rule may be overly cautious, leading to about 30% of tropical profiles being discarded. Further investigations may result in less draconian quality screening rules, to be described in the validation papers and the full data quality document.

O3 (stratosphere and mesosphere)

- Responsible scientist: Lucien Froidevaux (lucien@mls.jpl.nasa.gov)
- Useful range: 216 hPa (if in stratosphere) - 0.02 hPa

The main difference in the stratospheric O3 averages is a slight change in the slope versus pressure (or altitude). Globally, average values are now roughly 5% smaller near 100 hPa and about 10% larger near 1 hPa;

this helps to rectify small systematic differences that existed (to varying degrees) between v1.5 MLS data and correlative data sets for stratospheric ozone. For example, MLS ozone values for v2.20 data are typically within about 5% agreement with SAGE II coincident profiles, from 147 to 0.15 hPa. MLS version 2.20 stratospheric ozone columns (column values down to near the tropopause) are reduced in comparison to v1.5 ozone columns by roughly 1 to 3 DU (or about 0.5 to 1.5%), with the larger decreases obtained at high latitudes. There are 2 separate ozone columns (typically in very good agreement) in the L2GP O3 files, with swath names 'O3 column-MLS' and 'O3 column-GEOS5', corresponding to the use of tropopause pressures (WMO definition) determined from MLS or GEOS-5 temperatures, respectively. Better calibration of narrow digital autocorrelator spectrometer (DACS) channels now provides more confidence in the mesospheric ozone values. Negative precision values for ozone often occur at pressures lower than 0.02 hPa, indicating increasing influence from the a priori, although MLS information still exists (e.g., average day/night differences) in the uppermost mesosphere and lower thermosphere.

- Data screening:

Only use profiles with even values of Status and positive precision values, and with Quality > 0.4 and Convergence < 2.

H2O and RHi

- Responsible scientists:
  Troposphere/Lower Stratosphere: Bill Read (bill@mls.jpl.nasa.gov)
  Stratosphere/Mesosphere: Alyn Lambert (Alyn.Lambert@jpl.nasa.gov)
- Useful range: 316 - 0.002 hPa

H2O is now retrieved on a grid having 12 levels per decade change in pressure (~1.3 km spacing) from 316 hPa to 22 hPa. Minor spectroscopic changes (< 5%) have occured. Overall differences relative to v1.5 are small but individual levels near the tropopause can show large (about 20%) changes. This is mostly due to smoothing changes caused by halving the vertical grid. Water vapor values for pressures greater than 316 hPa are constrained to the results of a single layer relative humidity retrieval whose sensitivity peaks between 350 and 700 hPa. This is considered an improvement over the zonal-mean climatology used in v1.5. The estimated precisions for pressures greater than 100 hPa are much better than for v1.5. Version 2.20 now makes use of the DACS radiances and therefore extends the vertical range of H2O up to 0.001 hPa. The vertical resolution is 2.5 km at 150 hPa, 3 km at 100 hPa, and 3.5 km at 10 hPa. Horizontally it is 200 km. Preliminary comparisons with AIRS show excellent agreement (< 6% between 316 and 178 hPa) provided one

screens the data as given below, AIRS values are properly screened, and all AIRS data are rejected whenever MLS measures less than 20 ppmv. MLS v2.2 shows excellent agreement with the in situ CFH sondes in the tropical tropopause and lower stratosphere. Version 2.20 is greatly improved over the provisional v2.10 data in the tropical tropopause region (less noisy and spiky) and eliminates the moist bias introduced in the latter version throughout the stratosphere.

- Data Screening:

Only use profiles with even values of Status and positive precision values, and with Quality > 0.9.

- Artifacts:

As with v1.5, profiles with incorrectly dry values that pass the screening recommendations occur at 316 hPa. A different screening recommendation will need to be determined for this level. Comparisons with AIRS H2O results show that MLS mixing ratios greater than 500 ppmv are probably overestimated.

N2O

- Responsible scientist: Alyn Lambert (Alyn.Lambert@jpl.nasa.gov)
- Useful range: 100 to 1.0 hPa

The v2.20 N2O data show significant improvements over the v1.5 data, mainly through the use a more accurate forward model for the band 12 (N2O) radiances. The high biases seen in v1.5 N2O in the lower stratosphere (at 68 hPa and greater) in the polar vortex and near-vortex regions have been eliminated. Average values for v2.20 are 10% larger than v1.5 for pressures less than 50 hPa and at 100 hPa, they are 15% smaller and the initial comparisons with coincident N2O measuremements by ACE-FTS, Odin/SMR, and Envisat/MIPAS show smaller mean biases.

- Data screening:

Only use profiles with even values of Status and positive precision values, and with Quality > 0.5 and Convergence < 1.55. The poorly converged profiles (for this product) tend to stay very close to the a priori at 100 hPa and need to be rejected. This data screening rejects a few percent of the profiles globally, but significantly more (typically 5 to 10%) in the tropics. Clouds do not seem to have a significant impact (outside the noise) on N2O profiles at pressures down to 100 hPa.

- Artifacts:
The allowed N2O values have been restricted in the retrieval to a low bound of -40 ppbv (approximately three times the retrieval noise level in the recommended pressure range) in order to prevent a problem occuring in the minimization search process. The low bound is applied at all levels but it is only evident in the data for pressures less than 0.1 hPa where the N2O precision is of order 50 ppbv.

HCl

- Responsible scientist: Lucien Froidevaux (lucien@mls.jpl.nasa.gov)
- Useful range: 100 - 0.14 hPa

A slightly different set of channels (now from band 14) is used in the v2.20 retrievals for the standard HCl product, as a result of deterioration observed in nearby band 13 (originally used for v1.51 HCl) since early 2006. Band 13 has been turned off since Feb. 16, 2006, except for occasional days as a diagnostic. For days prior to this date, the MLS v2.20 software also produces a separate 'HCl-640-B13' product (stored in the L2GP-DGG file) using the band 13 radiances. This product has slightly better precision and vertical resolution than the v2.20 'standard' HCl product, but is only available up to Feb. 15 2006. MLS HCl data continuity across the Feb. 16, 2006 date requires v2.20 (reprocessed) standard HCl product data, as there are small (typically a few percent) discontinuities if one uses v1.51 data prior to that date, in conjunction with v1.52 data thereafter. Asside from these issues, the standard HCl product for v2.20 is noisier than v1.5 data, but has better vertical resolution in the upper stratosphere, mainly because of changes made to the retrieval's vertical smoothing constraints. HCl precision values are often flagged negative for pressures lower than 0.14 hPa, indicating increasing influence from the a priori, although MLS information still exists in the upper mesosphere. Overall, there are typically < 5-10% changes in the average HCl values, relative to v1.5 data; retrieved values are now slightly larger in the upper stratosphere and lower mesosphere, and smaller in the lower stratosphere. The differences versus HALOE and ACE-FTS HCl data are overall similar to those observed for v1.5 data [see Froidevaux et al., IEEE 2006 reference on early validation results, link available from the MLS website].

- Data screening:

Only use profiles with even values of Status and positive precision values, and with Quality > 1 and Convergence < 1.5. The poorly converged profiles (for this product) tend to stay very close to the a priori and need to be rejected. This data screening rejects a few percent of the profiles globally, but significantly more (typically 5 to 10%) in the

tropics.

ClO

- Responsible scientist: Michelle Santee (mls@mls.jpl.nasa.gov)
- Useful range: 100 - 1 hPa

The ClO data in v2.20 are for the most part similar to those in v1.5, with an estimated single-profile precision of about 0.1-0.2 ppbv throughout the vertical range. Similar levels of ClO enhancement are seen in the winter polar regions in the two datasets, but maximum mixing ratios near the secondary peak (2-3 hPa) in ClO are slightly smaller in v2.2. There is a pervasive negative bias of 0.4-0.5 ppbv (slightly larger than in v1.5) for the retrieval levels at and below 46 hPa; taking day/night differences largely eliminates this artifact. Vertical resolution is about 3 km in the lower stratosphere, degrading to about 4.5 km in the upper stratosphere. Horizontal resolution is < 10 km cross-track and about 250-350 km along-track throughout most of the stratosphere.

- Data screening:

Only use profiles with even values of Status and positive precision values, and with Quality > 0.8. This threshold for Quality is a conservative value that potentially discards a significant fraction of "good" profiles (while not necessarily identifying all "bad" ones) and may be revised after further investigation.

HNO3

- Responsible scientist: Michelle Santee (mls@mls.jpl.nasa.gov)
- Useful range: 147 - 3.2 hPa (215 hPa data may also be useful)

The HNO3 data in v2.2 are greatly improved over those of v1.5. Correction of a spectroscopy error has reduced mixing ratios by about 30%. Large oscillations in the retrievals have been mitigated, producing much more realistic behavior at pressures greater than 100 hPa. Scatter has been reduced and overall the profiles are much smoother, leading to an estimated single-profile precision of 0.5-1 ppbv throughout the recommended vertical range. Vertical resolution is about 3.5-4 km in the upper troposphere and lower stratosphere, degrading to about 6 km in the middle stratosphere. Horizontal resolution is about 10 km cross-track and 300-500 km along-track throughout most of the stratosphere. Preliminary analysis indicates that the v2.2 HNO3 retrievals at 215 hPa

may be useful for scientific studies, but further validation is necessary to confirm their reliability.

- Data screening:

Only use profiles with even values of Status and positive precision values, and with QUALITY > 0.5. This threshold for QUALITY is a conservative value that potentially discards a significant fraction of "good" profiles (while not necessarily identifying all "bad" ones) and may be revised after further investigation. It is also currently recommended that at and below 100 hPa (lowermost stratosphere and upper troposphere), all profiles with nonzero values for Status be discarded to mitigate potential cloud contamination; this criterion rejects a substantial fraction of profiles (30-40%) in the tropics and may be relaxed after more detailed analysis.

OH

- Responsible scientist: Herbert Pickett (Herbert.M.Pickett@jpl.nasa.gov)
- Useful range: 32 - 0.003 hPa

There are many beneficial changes in OH above 50 km. The profiles are smoother, have uniform 6/decade pressure resolution, and much fewer instances of negative concentration. In the stratosphere, OH fits are less subject to convergence problems and have better calibration, affecting accuracy by as much as 2%. From 32 to 10 hPa, one should use day - night differences to reduce biases.

- Data screening:

Only use profiles with even values of Status and positive precision values, and with Convergence < 1.1.

HO2

- Responsible scientist: Herbert Pickett (Herbert.M.Pickett@jpl.nasa.gov)
- Useful range: 21 - 0.02 hPa

The main change for HO2 is that there is more smoothing applied. The effect at altitudes below 60 km is to broaden the averaging kernel to 5 km FWHM in the vertical and 5 degrees along the track. Precisions are no longer flagged negative above 60 km (0.1 hPa) but it is estimated that there is at least 20% a priori contamination for altitudes above 0.32 hPa.

- Data screening:

Only use profiles with even values of Status and positive precision values, and with Convergence < 1.1.

BrO

- Responsible scientist: Nathaniel Livesey (livesey@mls.jpl.nasa.gov)
- Useful range: 10 - 2.2 hPa

As before, the BrO product requires significant averaging (e.g., monthly zonal mean) for scientific use. Indications are that the v2.2 software has reduced the persistent vertical structure in the v1.5 data that rendered the earlier data unusable. Significant biases are seen in v2.2 data at all altitudes in the stratosphere. These can be reduced by taking day/night differences. The usefulness of this product remains to be investigated.

- Data screening:

Only use profiles with even values of Status and positive precision values, and with Quality > 1.2 and Convergence < 1.6. The poorly converged profiles (for this product) tend to stay very close to the a priori and need to be rejected. This data screening rejects a few percent of the profiles globally, but significantly more (typically 5 to 10%) in the tropics.

HCN

- Responsible scientist: Hugh Pumphrey (H.C.Pumphrey@ed.ac.uk)
- Useful range: 10 - 0.1 hPa

Stronger smoothing constraints mean that the HCN product is now usable between 32 km (10 hPa) and 64 km (0.1 hPa). This product is still rather noisy, but much less so than in version 1.5. We do not recommend the use of this product for P > 10 hPa because of large systematic errors that are still present in this region.

- Data screening:

Only use profiles with even values of Status and positive precision values, and with Quality > 0.2 and Convergence < 2. Quality values are usually near 1.5; occasional lower values do not seem correlated with unusual profiles, but we suggest that profiles with Quality < 0.2 be rejected as a precaution (poorest radiance fits). Convergence is usually very close to 1.

HOCl

- Responsible scientist: Lucien Froidevaux (lucien@mls.jpl.nasa.gov)
- Useful range: 10 - 2 hPa

Average HOCl values for v2.2 data are generally somewhat lower (roughly 10% on average in the upper stratosphere) than for v1.5. There are still significant artifacts in the mean values (e.g., monthly zonal means) for this noisy product in the lower stratosphere, where it is not recommended for use.

- Data screening:

Only use profiles with even values of Status and positive precision values, and with Quality > 1.4 and Convergence < 1.5. The poorly converged profiles (for this product) tend to stay very close to the a priori and need to be rejected. This data screening rejects a few percent of the profiles globally, but significantly more (typically 5 to 10%) in the tropics. Also, band 29 (targeted for HOCl) was turned off for most days from March 29 through May 17, 2006. While some HOCl retrieval sensitivity is evident from nearby active bands, these retrieval days are not recommended for use.

SO2

- Responsible scientist: Bill Read (bill@mls.jpl.nasa.gov)
- Useful range: 147 - 10 hPa

SO2 is a new MLS retrieval, useful for monitoring volcanic injections into the stratosphere (MLS is not sensitive to background stratospheric amounts).

- Data screening:

Onlu use profiles with even values of Status and positive precision values, and with Quality > 0.5, in order to remove the largest fliers (and cases of most poorly fitted radiances).

CH3CN

- Responsible scientist: Michelle Santee (mls@mls.jpl.nasa.gov)

The v1.5 CH3CN data were not recommended for use in scientific studies,

and the usefulness of the CH3CN product in v2.2 remains to be investigated.

Cloud Ice Water Content (IWC)

- Responsible scientists: Dong Wu (dwu@mls.jpl.nasa.gov)
Jonathan Jiang (jonathan@mls.jpl.nasa.gov)
- Useful range: 261 - 68 hPa

The MLS ice water content (IWC) product (units of g/m3) is now recommended over a larger vertical range than the v1.5 IWC data. The IWC precision is generally improved over the v1.5 retrievals for pressures between 68 and 178 hPa, and, for high latitudes, down to the 261 hPa level as well. In addition, the number of false alarms (erroneous indications of cloud) is reduced for pressures < 178 hPa. The retrievals for large IWC values (which were underestimated in v1.5 data mainly for pressures > 147 hPa) have been improved. Also, a new cloud ice product, ice water path (IWP, units of g/m2), is now included in the standard IWC file as a separate swath. It is based on 240 GHz cloud-induced radiances from 650 hPa tangent pressure, and represents a vertical column above about 6 km.

- Data screening:

The same off-line procedure and thresholds as for v1.5 should be applied for cloud detection. However, no correction factors are needed for v2.2.